

On Effective Electron Mass of Silicon MOSFET at Low Electron Density.

V.T. Dolgoplov

Institute of Solid State Physics, RAS, Chernogolovka, 142432 Russia

The trial wave function method developed in Ref.s^{1,2} for the case of narrow s -band in a perfect crystal is adapted for calculation of the density dependence of the effective mass and the Lande factor in a dilute two-dimensional electron system. We find that the effective mass has a tendency to diverge at a certain critical concentration, whereas the g factor remains finite.

PACS numbers: 71.30.+h, 73.40. Qv

As the temperature decreases, a dilute electron gas of highly mobile Si-MOSFET exhibits a strong drop in the resistance if the electron density n_c is higher than a certain critical one $n_s > n_c$, and an increase in resistance when $n_s < n_c$ ³. In the vicinity of n_c the resistance possesses scaling properties as a function of temperature and electron density. This instance from the very first caused researchers to consider the observed transition as a disorder-controlled quantum phase metal-insulator transition (MIT) and gave rise to a tide of similar investigations of other systems in which any change in the sign of derivative $\frac{dR}{dT}(n_s)$ was taken as an evidence of the occurrence of a quantum phase MIT.

In the recent experimental study⁴ of the screening properties of a two-dimensional electron system as a function of temperature⁵, the interpretation was used in the terms of Ref.⁶, and a strong increase of the effective mass was found in Si-MOSFET as the electron density approached a value of $\sim 0.8 \cdot 10^{11} \text{ cm}^{-2}$, which is close to n_c in the best of investigated samples. A similar behavior of the cyclotron mass was observed in independent⁷ experiments on the measurement of the temperature dependence of Shubnikov-de Haas oscillations. An analysis of the experimental data similar to that made in⁴ but performed in the opposite limit in the ratio of valley-splitting energy to temperature with the use of data of other experimental groups and samples from other sources^{8,9}, confirmed the versatility of the $m^*(n_s)$ curve.

The conclusion that should be made from recent experimental data is that the quantum phase transition observed in the most perfect MOSFET is rather the property of a pure disorder-free two-dimensional system. A qualitative theory of two-dimensional electron Fermi liquid in a state close to crystallization was presented in Ref.s^{11,12}. Below a quantitative description of a two-dimensional paramagnetic electron liquid is proposed, adapting the trial wave function approach developed in Ref.s^{1,2} for the case of a narrow s band in a perfect crystal.

Let us assume that the ground state of an electron system with strong interaction in a regime close to crystallization can be described as an crystal with a great number of charge -carrying mobile defects. The real two-dimensional system will be replaced by a grid of lattice sites with a density of n_s . An electronic wave function of the Wannier type $\phi[(\mathbf{r} - \mathbf{g})n_s^{1/2}]$, where the vector \mathbf{g} specifies the position of a lattice site, will be associated with each site. The corresponding creation operator is $a_{\mathbf{g}}^\dagger$. If each site were occupied by only one electron, the system would represent a perfect electron crystal. In fact, there is a certain probability depending on n_s that in the ground state a site can be occupied by two electrons with opposite spins. The number of such states eventually determines the number of mobile excitations and, hence, the transport properties of the system.

Bloch wave functions are constructed on the base of lattice sites:

$$\psi_{\mathbf{k}}(\mathbf{r}) = n_s^{-1/2} \sum_{\mathbf{g}} \exp(i\mathbf{k}\mathbf{g}) \phi(\mathbf{r} - \mathbf{g}), \quad (1)$$

$$a_{\mathbf{k}}^\dagger = n_s^{-1/2} \sum_{\mathbf{g}} \exp(i\mathbf{k}\mathbf{g}) a_{\mathbf{g}}^\dagger. \quad (2)$$

The Hamiltonian of the system contains the electron kinetic energy and the electron interaction at one site:

$$H = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} (a_{\mathbf{k}\uparrow}^\dagger a_{\mathbf{k}\uparrow} + a_{\mathbf{k}\downarrow}^\dagger a_{\mathbf{k}\downarrow}) + \frac{\alpha e^2}{\varepsilon_0 n_s^{1/2}} \sum_{\mathbf{g}} a_{\mathbf{g}\uparrow}^\dagger a_{\mathbf{g}\downarrow}^\dagger a_{\mathbf{g}\downarrow} a_{\mathbf{g}\uparrow}. \quad (3)$$

Here, $\varepsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m}$, and ε_0 is the static dielectric constant. We introduced a coefficient α into the interaction energy determined by the exact form of the wave function on the site and completely neglected the electron interaction on the neighboring sites. Processing to the limit of the gas of noninteracting electrons requires the modulation in Eq.(1) disappear and the coefficient α be a slowly varying function of n_s , vanishing at $n_s^{-1} \rightarrow 0$. We will neglect this weak dependence in the region of a low electron densities.

In Ref. ¹, it was proposed that a many-body trial function be used for a ground state in the form

$$\psi = \sum_{G\Gamma} A_{G\Gamma} \prod_G a_{\mathbf{g}\uparrow}^\dagger \prod_\Gamma a_{\mathbf{g}\downarrow}^\dagger \Phi_0, \quad (4)$$

where G and Γ are the sets of sites occupied by electrons with spin up and down, respectively; and Φ_0 is a vacuum state. It is convenient to express the function ψ through operators of creation and annihilation of Bloch waves and to take into account electron correlation by decreasing coefficient $A_{G\Gamma}$ in (4) by a factor of η^ν if the corresponding product implies the occurrence of doubly occupied sites whose fraction equals ν ($0 < \eta < 1$). The relation between ν and η in the ground state was obtained in¹. For our case,

$$\eta = \nu \left(\frac{1}{2} - \nu \right)^{-1}. \quad (5)$$

The probability that a single-particle state with a wave vector \mathbf{k} is occupied undergoes a jump at $k = k_F$ by the value

$$q = 16\nu \left(\frac{1}{2} - \nu \right). \quad (6)$$

Thus, the trial wave function describes a mixture of functions that corresponds to a fully occupied band (solid spin-ordered phase) and a paramagnetic electron liquid. The transition to the solid phase is continuous and is characterized by the parameter q ($0 \leq q \leq 1$): $q = 1$ in the paramagnetic electron liquid with weak interaction, and $q = 0$ in the electron crystal.

The mean value of the Hamiltonian given by (3) in the state with given ν equals

$$\langle H \rangle_\nu = \frac{1}{2} n_s q \varepsilon_F + \nu \frac{\alpha e^2}{\varepsilon_0} n^{3/2}, \quad (7)$$

where ε_F is the Fermi energy of an equivalent number of electrons in the absence of interaction. According to², the expression in Eq. (7) is minimized with respect to ν with regard to Eq.(6). A minimum of the Hamiltonian is attained at

$$\nu = \frac{1}{4} \left(1 - \left(\frac{n_{c1}}{n_s} \right)^{1/2} \right); n_{c1} = \left(\frac{\alpha e^2 m}{2 \varepsilon_0 \pi \hbar^2} \right)^2; \quad (8)$$

which, according to (6), corresponds to

$$q^{-1} = \frac{m^*}{m} = \frac{n_s}{n_s - n_{c1}}. \quad (9)$$

Here, m^* is the renormalized effective mass. In the same way, following², the Lande factor can be found as

$$\frac{g^*}{g} = \left[1 - \left(\frac{n_{c1}}{n_s} \right)^{1/2} \frac{1 + \frac{1}{2} \left(\frac{n_{c1}}{n_s} \right)^{1/2}}{\left(1 + \left(\frac{n_{c1}}{n_s} \right)^{1/2} \right)^2} \right]^{-1}, \quad (10)$$

The simplest way of generalization to the case of two valleys is in considering two parallel sublattices. In each of them the number of electrons equals $n_s/2$ and the characteristic cell size is diminished compared to the single-valley case by a factor of β . The coefficient β is determined by the ratio of Coulomb energies of inter and intravalley interactions. In the limit of two sublattices in one plane $\beta = \sqrt{2}$. In the case of two valleys, n_{c1} in Eq. (9,10) should be replaced by $n_{c2} = 2\beta^2 n_{c1}$.

A comparison of the curves obtained in this way with experimental results is shown in Figs. 1,2. Single fitting parameter $n_{c2} = 0.78 \cdot 10^{11} \text{ cm}^{-2}$ has been used, which corresponds to $\alpha = 0.15$. It is evident from the figures that the behavior of both the effective mass and the g -factor is reasonably described within framework of the proposed model, though the coefficient α is approximately twice as large as the value expected according to numerical calculations¹⁰.

It should be specially noted that the above considerations give no way of judging the spin state of the solid phase, because it is determined by the exchange interaction of electrons on neighboring sites. Moreover, in the immediate vicinity of the transition point, in the region where $(\langle H(n_s) \rangle_\nu - \langle H(n_c) \rangle_\nu) n_s^{-1}$ turns out to be smaller than the exchange energy of electrons on neighboring sites, the proposed description does not work in the paramagnetic electron liquid as well. Thus, the issues of the phase diagram in the immediate vicinity of the transition point and those of the spin structure of the solid phase remain out of scope of this consideration. In general, the approximation used is poorly controlled, and the rather good description of experiment still remains its only justification.

It is well known that the concentration n_c that corresponds to a change of the sign of the derivative dR/dT strongly varies from sample to sample, depending on the disorder in the electron system under study. An impression is gained from experimental data that the transition point n_{c2} measured for different samples also somewhat varies. This fact can also be related to the effect of disorder, as was discussed in^{11,12}. In strongly disordered electron systems $n_c \gg n_{c2}$ and the effect considered above, namely, the dramatic increase in the effective mass is not observed. In the most perfect of the electron systems studied, $n_c \approx n_{c2}$.

Author is grateful to V.F. Gantmakher, A. Gold, S.V. Iordanski, B. Spivak, D.E. Khmelnitskii, and A.A. Shashkin for useful discussions. A significant part of this work was carried out at the LMU, and the author is grateful to J.P. Kotthaus and researchers from his institute for help and discussions.

This work is supported by the Russian Foundation for Basic Research, the Ministry for Science and Technology of the Russian Federation, and by A. von Humboldt Forschungspreis.

-
- ¹ M.C. Gutzwiller, Phys. Rev. **137**, A1726 (1965).
² W.E. Brinkman and T.M. Rice, Phys. Rev. B **2**, 4302 (1970).
³ E. Abrahams, S. V. Kravchenko, and M. P. Sarachik, Rev. Mod. Phys. **73**, 251 (2001).
⁴ A.A. Shashkin, S.V. Kravchenko, V.T. Dolgoplov, and T.M. Klapwijk, Phys. Rev. B **66**, 073303 (2002).
⁵ A. Gold, and V.T. Dolgoplov, Phys. Rev. B **33**, 1076 (1986).
⁶ Gabor Zala, B.N. Narozhny, and I.L. Aleiner, Phys. Rev. B **64**, 214204(2001).
⁷ V.M. Pudalov, M.E. Gershenson, H. Kojima, M. Butch, E.M. Dizhur, G. Brunthaler, A. Prinz, and G. Bauer, Phys. Rev. Lett. **88**, 196404 (2002).
⁸ S.A. Vitkalov, K. James, B.N. Narozhny, M.E. Sarachik and T.M. Klapwijk, cond-mat/0204566.
⁹ V.M. Pudalov, M.E. Gershenson, H. Kojima, G. Brunthaler, A. Prinz and G. Bauer, cond-mat/0205449.
¹⁰ B. Tanatar and D.M. Ceperley, Phys. Rev. B **39**, 5005 (1989).
¹¹ B. Spivak, Phys. Rev. B **64**, 085317 (2001).
¹² B. Spivak, cond-mat/0205127.
¹³ V.M. Pudalov, M.E. Gershenson, and H. Kojima, cond-mat/0110160.

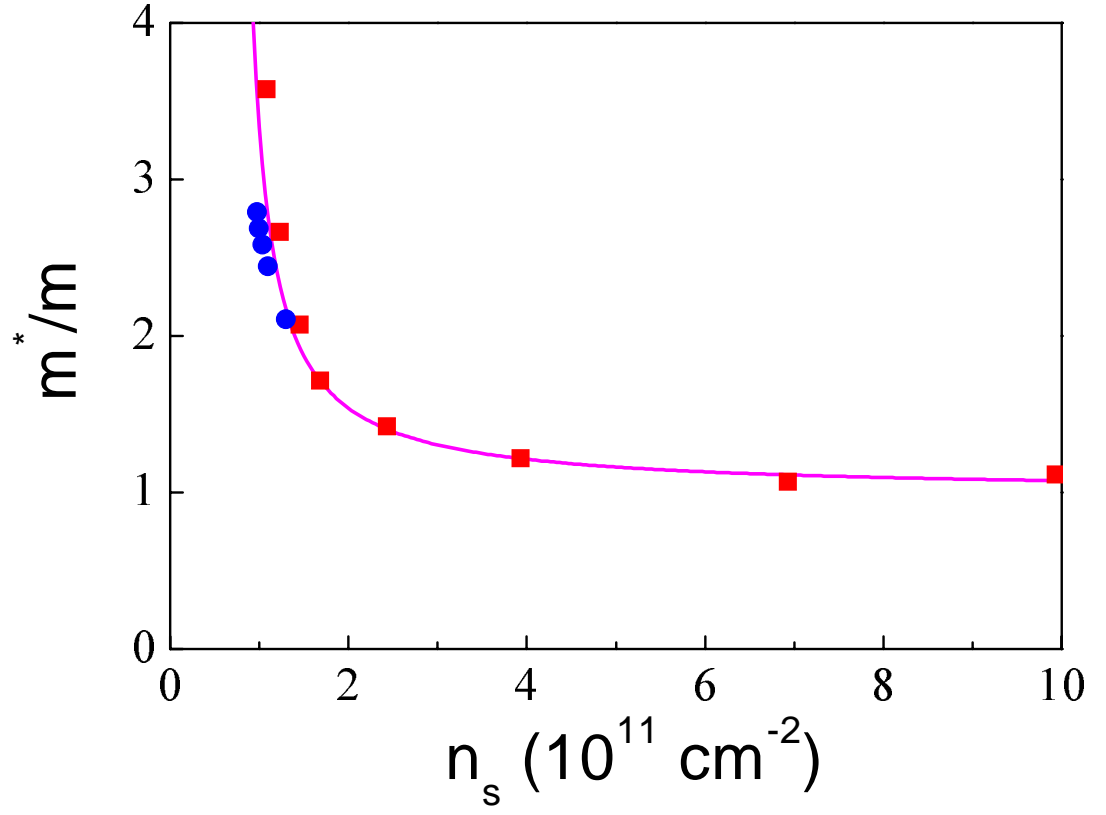


FIG. 1. Effective mass as a function of electron density. The solid line corresponds to Eq. 9 with $n_{c2} = 0.78 * 10^{11} \text{ cm}^{-2}$. Squares and circles correspond to the experimental data from Ref.⁴, and Ref.¹³, respectively.

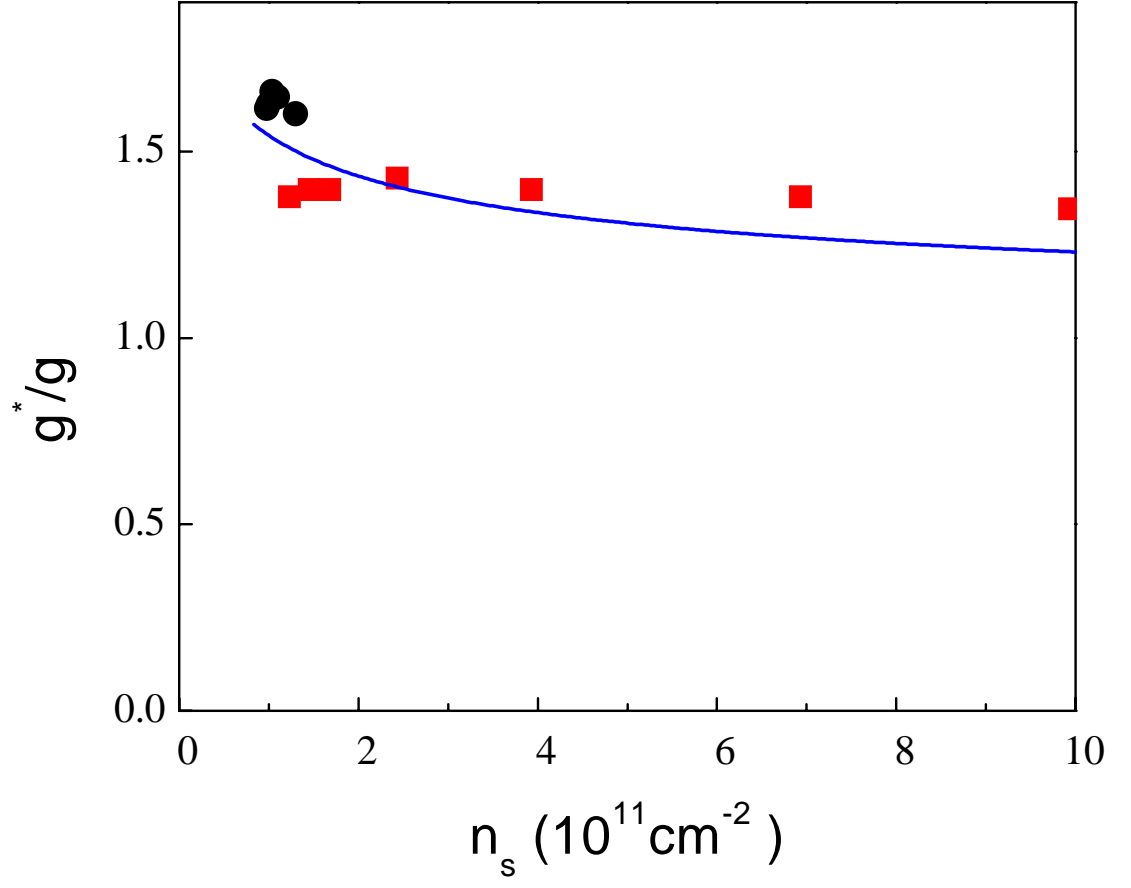


FIG. 2. Effective g -factor as a function of electron density. The designations of experimental points are the same as in Fig. 1.